N,N-Diethylaniline

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 5.97e-11 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.33e-01

Confidence level: 8.62e-01

Nearest Neighbors from the Training Set

Image not found
1,3,5-Cycloheptatriene
Measured: 9.69e-11
Predicted: 1.00e-10

Image not found
(2E)-3-Phenylprop-2-enal
Measured: 4.80e-11
Predicted: 5.31e-11

Image not found
(2E)-2-Hexenal
Measured: 4.40e-11
Predicted: 4.31e-11

Image not found
2-Methyl-p-benzoquinone
Measured: 2.35e-11
Predicted: 2.15e-11

Image not found
Cyclohepta-1,3-diene
Measured: 1.39e-10
Predicted: 1.35e-10